Splendor and Misery of Chasing Optimality

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According to the Wikipedia, computational science or scientific computing is the field of study concerned with constructing mathematical models, quantitative analysis techniques and using computers to analyze and solve scientific (real-world) problems. In practical use, it is typically the application of computer simulation and other forms of computation to problems in various scientific disciplines. It combines various tools from engineering and applications, applied mathematics, numerical analysis, matrix computations and parallel. Typically such mathematical models require massive amount of floating point calculations and are executed on modern distributed computer architectures. Such process can be seen as a sequence of several steps or subtasks that starts with certain experimental observation or measurements, and leads to appropriate mathematical description, often described by a system of some equations. This continuous model is usually further reformulated and approximated with a discretization technique resulting into algebraic problem solved by some linear algebra code properly implemented on a chosen computer architecture.

In this contribution, we want to look at one important and often neglected aspect of this whole process. It seems quite natural that one should make an effort and try to execute above mentioned steps in an optimal way. The notions of ideal measurement or exact data, perfect model, optimal solution, perfect scalability or exact solver are nice examples of the trend which can be hidden behind more general modern term: optimality. On the other hand, it is clear that for most realistic real world situations the optimality is not achievable and in the cases where the optimal solution does exist it cannot be found easily even by very efficient solution techniques. Therefore, in practice we often talk about data with noise, simplification of the model, approximations, discretization errors, algebraic error or roundoff. But is the optimality always desirable? Do we really want to spend time and resources to solve some subproblem to a high accuracy when it is not necessary? We illustrate our point on a few examples of ill-conditioned or ill-posed problems, including such linear algebra problems as matrix inverse, orthogonalization or solution of sets of equations using iterative Krylov subspace methods.

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